

Preface

In the past decade alone, we have witnessed enormous advancements in nanoscience and nanotechnology that promise to lead to revolutionary biomedical applications in drug delivery, optical imaging, biosensing, and nanotherapeutics. Accompanying this explosion of innovation, however, there are growing concerns about the biocompatibilities of nanomaterials central to these novel technologies. Many such nanoparticles are known, in specific contexts, to be acutely toxic to humans and detrimental to essential components of our environment. Prior to their broad implementation, it is therefore imperative to assess the deleterious effects these new and exciting technologies might exact on human and environmental health. Given the inherent complexity of nanoparticle–biomolecular interactions, a combined approach featuring state-of-the-art experimental and theoretical techniques is needed to address critical issues involving nanotoxicology at the “bio-nano-med” interface.

In parallel with nanotechnological advances, molecular modeling capabilities have rapidly progressed alongside improvements in simulation algorithms and unceasing augmentations to high performance computing resources. Enhancements to both experimental and computational techniques have dramatically narrowed the gap between the timescales that can be accessed through computer simulation and physical observation. Scientists can now probe microsecond- to millisecond-long processes in atomic detail, spatiotemporal resolution that is sufficient for characterizing many important interactions between nanoparticles and biomolecules (i.e., bionanomachines). This book aims to capture perspectives on the emerging field of “nanotoxicity modeling,” from its basis in theoretical nanochemistry to its ultimate realization in molecular and medical biology. The chapters, organized according to the type of nanomaterial each features, illustrate how molecular (classical mechanical) and atomic (quantum mechanical) modeling approaches can be applied to bolster our understanding of nanotoxicology. Together, these chapters provide a comprehensive overview of the fundamentals of nanotoxicity modeling and its implications for the development of novel nanomedicines.

Until now, progress toward conducting large-scale molecular dynamics simulations has been led by a small group of risk-takers. Although molecular modeling techniques have existed for some time, recent groundbreaking advancements in massively parallel supercomputers and novel parallelization algorithms have thrust the field of physics-based simulation into an exciting regime of broad accessibility. As evidenced by the foci of the Nobel Prize in Chemistry in 2013 and many new conferences around the world, interest in molecular modeling is more pronounced than it has ever been. Leveraging the maturity of molecular simulation algorithms and techniques, this readily accessible text lays out the fundamentals of nanotoxicity modeling for an array of nanomaterial systems, ranging from carbon-based nanoparticles to noble metals, metal oxides, and quantum dots. I sincerely hope this book serves to extend practical knowledge to a large community that can aid biocompatibility assessment efforts in a coming age of nanotechnology.

This book discusses advanced techniques with real-world examples of nanotoxicity modeling for various types of nanomaterials—content that should be useful to senior undergraduate students, graduate students, and established researchers in nanoscience, nanotechnology, nanotoxicology, nanomedicine, chemistry, physics, molecular biology, and computer science. Courses such as Nanotoxicology, Nanomedicine, Computational Chemistry, Biophysical Chemistry, Biophysics, Statistical Mechanics, and Computational Molecular Biology may find some of the content useful as primary or supplementary material. Additionally, this book may also be of interest to academic and industry professionals working on nanodrug discovery and related biomedical applications.

Finally, I would like to thank Dr. Jeffrey K. Weber, Tien Huynh, Dr. Camilo A. Jimenez-Cruz, Dr. Seung-gu Kang, Dr. Hongsuk Kang, Dr. Bruce Berne, and Royce W. Zhou for their careful reading of this book's chapters. I would also like to thank Editor Marta Moldvai for her patience and technical assistance during the preparation of this text. It would be impossible to put together this book without such generous help.

June 2015

Ruhong Zhou

Modeling of Nanotoxicity
Molecular Interactions of Nanomaterials with
Bionanomachines

Zhou, R.

2015, XIII, 189 p. 61 illus., 56 illus. in color., Hardcover

ISBN: 978-3-319-15381-0